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Sunset-calc: An R Shiny Application for Processing Thermo-Optical Analysis Data from Atmospheric Aerosol Measurements

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INTRODUCTION

- Atmospheric aerosols have adverse effects on human health[1]
- Atmospheric aerosols are emitted from natural and anthropogenic sources[2]
- Radiocarbon (^{14}C) is a naturally occurring radioactive ($t_{1/2}$ = 5730 years) isotope constantly formed in the upper atmosphere
- Source apportionment with ^{14}C can unequivocally separate biogenic from fossil-fuel derived sources
- Thermal-optical analysis aims to separate non-refractory organic carbon (OC) from refractory elemental carbon (EC)

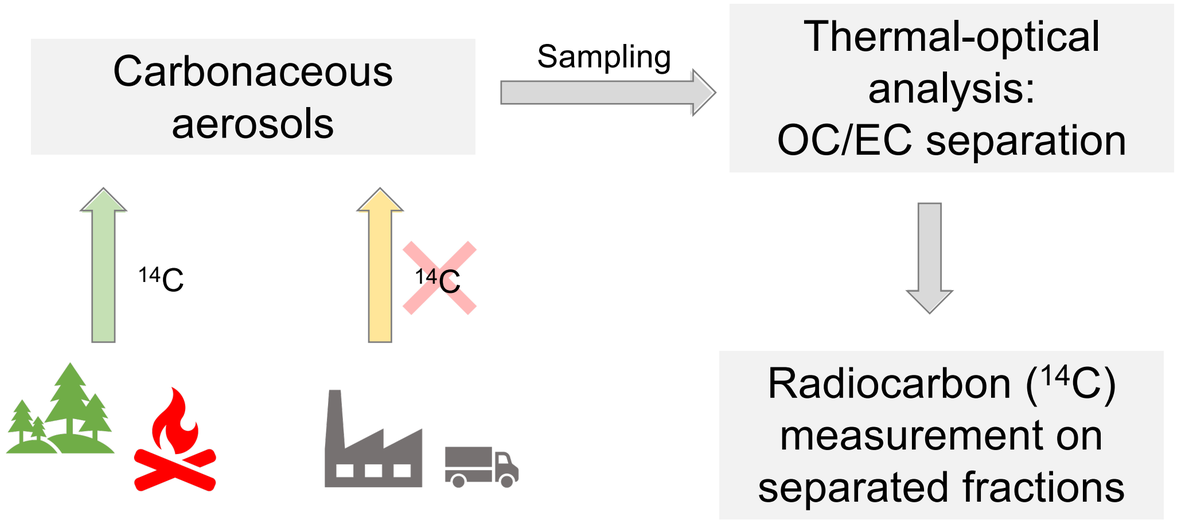

Fig. 1: From aerosol emissions to a radiocarbon measurement. *Aerosols from biogenic emissions and biomass combustion processes contain ^{14}C, whereas aerosols from fossil-fuel combustion are completely devoid of ^{14}C. Thermal-optical analysis separates organic carbon (OC) from elemental carbon (EC) before radiocarbon measurement.*

METHOD

- A Sunset thermal-optical analyser is used for the physical separation of OC and EC
- The OC/EC separation is monitored by a laser and a non-dispersive infrared (NDIR) detector

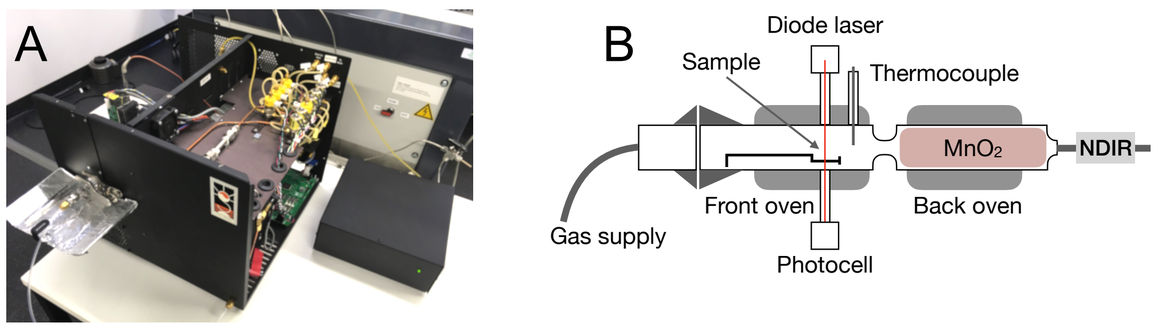

Fig. 2: Thermal-optical analyser. A: *Sunset OC/EC analyser with non-dispersive infrared (NDIR) detector on the right.* ***B:*** *Scheme of the sample oven in the Sunset OC/EC analyser with a laser for OC/EC separation monitoring.*

- Some OC is converted into EC (charring)
- Some EC is lost, which leads to a reduced EC yield
- Charring and EC yield must be optimised using the temperature for each aerosol filter campaign
- These artefacts must be corrected for

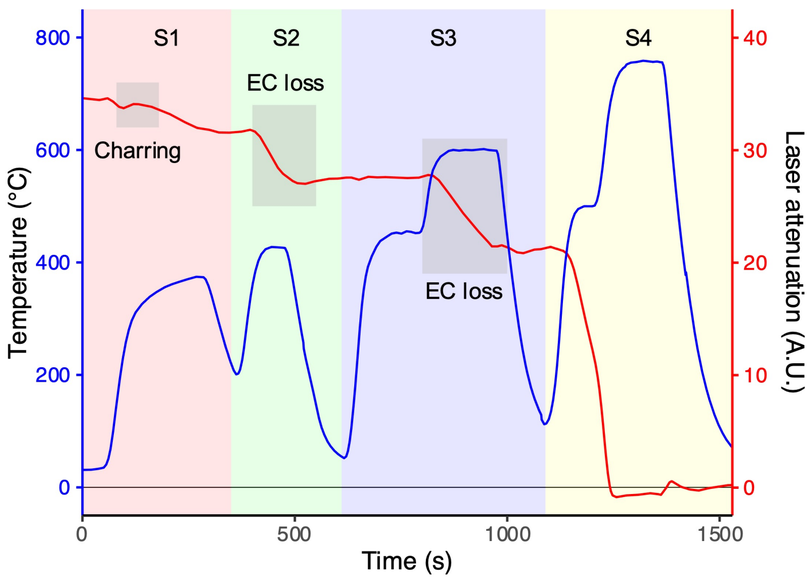

Fig. 3: Thermal-optical analysis. *Temperature and laser attenuation signal with a 4-step (S1 to S4) OC/EC separation protocol where S1 is pure OC and S4 is pure EC.*

GOAL AND MOTIVATION

- Improve processing of thermal-optical analysis data
- Excel spreadsheets were previously used
- Analysis was time-consuming and complicated with compatibility issues and various template versions

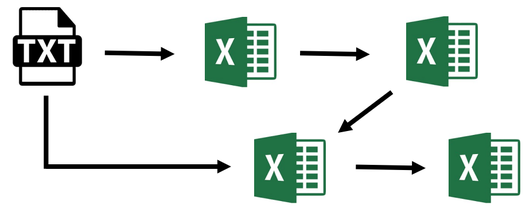

Fig. 4: Previous workflow. *Several Microsoft Excel spreadsheets were used for data analysis.*

RESULTS

- Data analysis from spreadsheets was rewritten and extended in R
- R Shiny was used to build a web application
- The Sunset-calc[3] application was deployed on an R server
- Sunset-calc provided instant benefits:
  - Calculation of EC yield and charring with visualisations
  - Corrected carbon amount calculation for custom protocols
  - Tedious & time-consuming spreadsheets replaced with drag and drop and almost instant results
  - User and platform independent and with version control

Fig. 5: Sunset-calc logo.

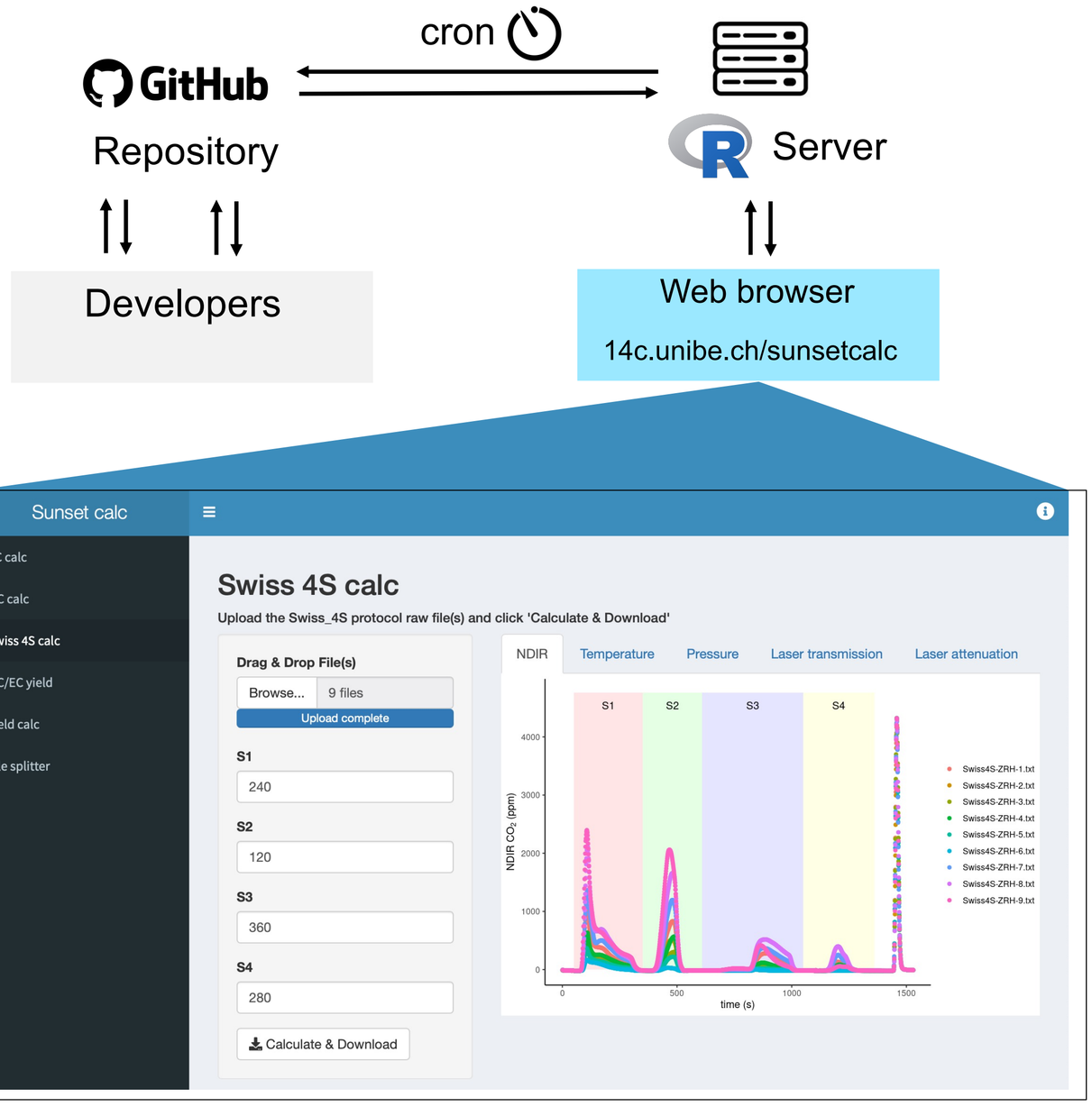

Fig. 6: Sunset-calc server deployment and user interface. *The desired analysis is selected in the menu and the analyser raw data files are uploaded in the web interface. The calculation results are provided as a download. Changes to Sunset-calc in the repository are automatically deployed to the R server.*

CONCLUSION

- Sunset-calc simplified and streamlined the lab workflow with automated data evaluation
- R with R Shiny provides a simple solution to create web applications suitable for people with little prior programming skills

References: [1] O. Boucher, Springer, 2012. [2] E. A. G. Schuur *et al.*, Springer, 2016. [3] github.com/martin-rauber/sunset-calc